# SAAM II Version 2.2 Basic Tutorials

## **Getting Started with Compartmental**

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### **Getting Started with SAAM II Compartmental**

#### Prerequisites

This tutorial has no prerequisites. It assumes you know the basics of the Windows operating system. It also assumes you have **SAAM II's Compartmental** application, version 2.2, installed on your computer, and that you know how to open the application.

#### What you will learn in this tutorial

The basic operations of the SAAM II Compartmental application:

- How to use a **SAAM II Compartmental** study file.
- How to use **SAAM II Compartmental** computational features.
- How to view solutions.
- How to build a model using the model building tools.
- How to create an experiment on the model using the experiment tools.
- How to enter data, and associate data with samples
- How to enter your model parameters.

#### **Files Required**

Study Files: The study file for the Compartmental application is

#### study\_0.stu

This file is included as part of this tutorial. This file is the same as **study\_0.stu** that is installed in the **SAAM II** program folder, and referred to in the **SAAM II** tutorials.

Data File: The data file for this tutorial is

#### study\_0.dat

The data file is a text file. (This file is the same as study\_0.dat that is installed in the **SAAM II** program folder, and referred to in the **SAAM II** tutorials.)

#### Introduction

This tutorial will show you how to perform the basic operations in the **SAAM II Compartmental** application. It is intended to help the new user get started quickly with **SAAM II** version 2.2.

This tutorial is divided into two parts. In the first part, you will load an existing **SAAM II** file. The purpose is to familiarize you with the basic computational operations, and how to view information from solutions. In the second part, you will build a model. This will familiarize you with the tools used to build models and create experiments.



In this **SAAM II** tutorial, special information or notes to assist the user in using the **Compartmental** application are preceded by the **Compartmental** symbol on the left and end with the small **Compartmental** symbol.



This part of the tutorial will show the key components of the model of a system and an experiment on the system, and the fundamental operations of **SAAM II** - solving, fitting, and viewing solution. You will work with the following two-compartment model.





*Transfer coefficients.* The **SAAM II** convention for the transfer coefficients k(i,j) is k(to,from). Thus k(2,1) is the transfer rate to Compartment **2** from Compartment **1**. The transfer rate k(0,1) is the rate of irreversible loss from Compartment **1**. The input arrow **U(1)** is for system experiments in tracer-trace experiments; this will not be discussed in the tutorial.



- 1. Start the SAAM II Compartmental application.
- 2. Open the SAAM II Compartmental study file study\_0.stu.

The file **study\_0.stu** should appear in the file list; if it does not, find the folder where you put this file.

In the File menu, click Open.

The **SAAM II Compartmental** main window will open as shown below:



The model shown on the **Drawing Canvas** is the **SAAM II Compartmental** representation of a two-compartment model. In **SAAM II** terminology, it is called the **System Model**; it is a mathematical representation of how the system functions, and is normally used to interpret tracee data in a tracer-tracee experiment.

The SAAM II Compartmental main window consists of four main areas:

The Menu bar:

File Edit View Show Compute Set Window Help

This menu bar contains the SAAM II menu items.

Below the Menu bar is the SAAM II Toolbar:

This toolbar contains **SAAM II** specific tools such as "Solve" or "Fit." Most of the toolbar functions can be found in the **Show** and **Compute** menus.

The Drawing Canvas will appear in part as follows:



The **Drawing Canvas** contains the area for building models and creating experiments using tools in the **SAAM II Toolbox**.

The SAAM II Toolbox:



The SAAM II Toolbox will be discussed in detail in the next part of this tutorial.

Take a minute to examine the various tools on the **SAAM II Toolbar** and in the **Toolbox**. Place the cursor on top of a **SAAM II** tool to show text describing the tool's function.

3. As you proceed through this tutorial, you will notice that several windows can be open at one time; this is normal and as you will see can be very helpful. An example is shown as follows:

SAAM II Compartment	al - STUDY_0.STU	
File Edit View Show Co	mpute Set Window Help	
	FIG MERZ @ZC 82	
Toolbox	K STUDY_0.STU:1	
Model	Image: Statistic statis statis statistic statistic statistic statistic stat	Plot 10 <sup>3</sup> 10 <sup>4</sup> 10 <sup>4</sup> 0.21472 2408.65103 V

In most cases in this tutorial, only the current window will be shown in the text. In the actual application, several windows may actually be open.

4. Dialog boxes associated with **SAAM II** objects.



*Objects and dialog boxes.* Every object on the **Drawing Canvas** has a dialog box associated with it.

- တ်းစာ လေးမျ
  - a. To open the dialog box associated with a particular object, simply double-click that object. For example, if you double-click Compartment 1, the Compartment Attributes dialog box for Compartment 1 will open as shown below:

Compartment Attributes	×
Compartment Number: 1	
Reference Name:	
Done Cancel Help	

There is a box with the compartment number in it, and a box to add a reference name. If you wish, you can change the compartment number, or you can add a reference name such as "Plasma." The reference name will appear in the circle that represents Compartment 1; it is for reference purposes only and is not used by the software.

- b. To close the dialog box, click **Done**.
- 5. Open and investigate the experiment on the System Model.



*Models of systems and models of experiments:* It is very important to understand the **SAAM II** philosophy of separating the creation of the system model, i.e. how you believe your system functions in terms of a compartmental model, from duplicating an actual laboratory experiment on the model. As you will learn in Part 2, the **Model** tools in the **SAAM II Toolbox** allow you to build a model for the system, and the **Experiment** tools in the **SAAM II Toolbox** allow you to create an experiment on the system model.



a. In the **SAAM II Toolbox**, click **Experiment**. The **SAAM II Compartmental** main window should appear as follows:



This is the model of the experiment. Notice that the compartment names have changed from 1 and 2, to q1 and q2. In SAAM II, q1 and q2 represent the differential equations created internally and solved by SAAM II. The input is the

experimental input syringe, **ex1**, and there is a sample icon, **s1**, representing the experiment sample.

b. On the **Drawing Canvas**, double-click **ex1**. The **Exogenous Input** dialog box will appear as follows:

Exogenous	Input					X
Name: ex1	1	Refe	rence		Units:	
Туре	Initial	Constant	Start	Stop	Repeat Every	Nr. Repeats
Bolus	1.04e+	8 -	0.000		125 C	-
-Input T	ype:	_	Initial Am	iount: 1.0	0400000e+008	□Save
• Bol	lus		Constant	Rate: 0.0	)	
C Inf	ับรion med Infusion		Event	Start: 0.0	)	⟨⊐Edit৶
C Equ	uation		Event	Stop: 0.0	)	<b>一Add</b>
			Repeat E	very:		
			Nr. of Rep	eats:		Delete 🕁
Equation:	ex1 =					
Split I	input		Do	one	Cancel	Help



*Experiment inputs.* There are many useful options for experiment inputs that you can specify in this dialog box. Several different types of input are possible: bolus, infusion, primed infusion, equation-described, repeated inputs, and split inputs. For this tutorial, a single bolus injection of 1.04e+08 dpm (disintegrations per minute) is being used.



- c. To close the dialog box, click **Done**.
- d. On the **Drawing Canvas**, double-click **s1**. The **Sample Attributes** dialog box will open as follows:

ample Attributes	
Name:	s1
Units:	dpm/mL
Associate with Data Name:	plasma
s1 = q1/vol	*
	T



*Sample Attributes*. There are many useful options for the experimental sample that you can specify in this dialog box.

The units of the experimental data, in this case dpm/ml, are for reference purposes only.

The **Associate with Data Name** box contains the name of the data in the data file associated with this sample. If you do not have a data name associated with a sample, and try to fit the model to the data, **SAAM II** will generate a warning message.

The sample equation in the **Equations** pane, in this case "s1=q1/vol", is the equation which links the solution of the differential equation **q1** with the data. Writing the sample equation is a fundamental step in building a model and adds a new parameter, *vol*, to the model.



- e. To close the dialog box, click **Done**.
- 6. View the data.

Data in **SAAM II** are entered in a text file where columns are space delimited. The data file for the study **study\_0.stu** can be viewed as follows:

a. In the **Show** menu, click **Data**, or alternatively, on the **SAAM II Toolbar** click **Data** The **Data** window will open as follows:

DATA (FSD 0,	1)	
t	plasma	
0.007	46780	
0.042	43522	
0.125	42535	
0.25	40125	
0.375	36221	
0.5	35562	
1.0	28194	
2.0	19573	
3.0	14403	
4.0	11278	
5.0	8081	
6.0	6999	
7.0	5653	
8.0	5139	
9.0	4210	
END		
100125		
and the second		
4		*

The first line of the data file is the word "DATA." The next line, (FSD 0.1) specifies the weights assigned to the data. The first column in the data file is always the independent variable, usually time denoted **t**. The columns representing data can be named whatever you wish; the name is case sensitive. However, the name of this column must be the same as the name in the appropriate **Sample Attributes** dialog box.



*Data weighting*. Data weighting is used to provide a measurement of the user's confidence in a particular datum and is used in the "fitting" process. Data weights are calculated as the inverse of the data variance. **SAAM II** contains several variance models. If no method is explicitly specified, a fractional standard deviation of 0.1 (FSD 0.1) is assigned as the variance model to each datum.

**SAAM II** calculates weight for each datum from the standard deviations you assign to your data. In the file above, the variance model, (FSD 0.1), means that a constant coefficient of variation (fractional standard deviation) of 10% is assigned to each datum. Therefore, for example, the standard deviation of the datum of 46780 is 4678.



- b. Close the Data window.
- 5. View the model parameters.

The model has four parameters: k(2,1), k(1,2), k(0,1) and vol. These parameters are entered in the **Parameters** dialog box.

a. In the **Show** menu, click **Parameters**, or alternatively, on the **SAAM II Toolbar** click **Parameters**. The **Parameters** dialog box will open as shown below:

<b>P</b> arameters				
Name	Туре	Current	Low Limit	High Limit
k(0,1)	Adj	0.1000	0.0100	1.0000
k(1,2)	Adj	0.1000	0.0100	1.0000
k(2,1)	Adj	0.1000	0.0100	1.0000
vol	Adj	2000.0000	200.0000	20000.0000
Name: k(0, 1)				
	Va	lue: 0.100000	00	⊐Editピ
Type: C Fixed	Low Li	mit: 0.010000	00	- A
Adjustable	High Li	mit: 1.000000	00	Save
Adjust value:				
_^_				
				Auto solve
Done	Cancel	Help		



*Properties of parameters.* There are several important features of the **Parameters** dialog box.

- i. Each parameter has a "Type" that is either "fixed" or "adjustable." A fixed parameter is a parameter that is assumed to be known and does not change when the model is "fitted" to the data. An adjustable parameter is adjusted when model is "fitted" to the data.
- ii. Each parameter, whether fixed or adjustable, has a "current" value; this is the value that will be used when you Solve or Fit the model.
- iii. Adjustable parameters have upper and lower limits. These are limits that cannot be exceeded when SAAM II Fits the model to the data. If SAAM II is Fitting the model to the data and a limit is reached, SAAM II will display a warning message.

- iv. To change a parameter value, double-click on the parameter name. Its current value, and high and low limits if it is adjustable, will be shown in the Value, High Limit and Low Limit boxes respectively. To save the changes, click Save.
- v. There is an "adjust value" slider bar that lets you adjust the value of a specific parameter by simply moving the slider button to a different location on the bar.



- b. To close the **Parameters** dialog box, click **Done**.
- 6. Solve the model.
  - a. In the **Compute** menu, click **Solve**, or alternatively, on the **SAAM II Toolbar** click **Solve**.



*Solve*. When you "Solve," **SAAM II** uses the current values of the parameters to solve the system of differential equations represented by the compartmental model.

During a "Solve," a **Solve Status** message will appear showing the status of the integration (solving). For small models such as this one, the message will appear and disappear extremely fast. For larger models, you can watch the progress. You can also choose to abort a "Solve."

## 

- 7. View the solution to the model using **Quick Plot**.
  - a. On the Drawing Canvas, click s1 to select it.
  - b. In the **View** menu, click **Quick Plot**.

The following plot will appear in the Quick Plot window. Notice that the scale is linear.





*Quick Plot.* **Quick Plot** has preset defaults that you cannot change. As you can see below, when you use the **Plot** command, you have more flexibility in what you can plot and how you can plot it.



c. To view this plot in semi-logarithmic mode, in the **View** menu, click **Semilog**. The plot will appear as follows:



d. Close the Quick Plot window.

- 8. View the solution to the model using the **Plot** command.
  - a. In the Show menu, click Plot, or alternatively, on the SAAM II Toolbar click Plot
    Image: The Plot and Table Variables dialog box will open as follows:

s1 : plasma	X-Axis j
	Select up to 10 Y-Axis Variables in List.
	Current Selection :

Only the variables that are associated with data will appear in the **Variables for Y-Axis** pane. However, you can plot any of the variables in the model as described below.

b. In the **Plot and Table Variables** dialog box, select the **List All Variables** check box. All the variables that can be plotted will appear as follows:

ariables for Y-Axis	X-Axis t
ex 1.bolus ex 1.infusion flux(0, 1) flux(1, 2) flux(2, 1) k(0, 1) k(1, 2) k(2, 1) plasma	Select up to 10 Y-Axis Variables in List. Current Selection :
q1 q2 s1_res s1_wres t_ vol	

You can now select among the different variables for the Y-Axis for the plot.

- c. In the **Plot and Tables** dialog box, clear the **List All Variables** check box to clear the Y-Axis variables except **s1:plasma**.
- d. In the **Variables for Y-axis** pane, click **s1:plasma**. The selection will move to the **Current Selection** pane.
- e. Click Done.

A plot similar to the previous **Quick Plot** will appear.

9. Change the plot variables.

**SAAM II** will remember the plot variables, e.g. **s1:plasma** when you open and shut the **Plot** window. If you want to change the plot variables, you need to change the variable names using the **Plot and Table Variables** dialog box in the **Set** menu while a **Plot** window is open. The following will illustrate how to plot **q1** and **q2** so you can compare the model solution for these two variables.

- a. With the **Plot** window open, in the **Set** menu, click **Plot/Table Variables**. The **Plot and Table Variables** dialog box will open.
- b. Select the List All Variables check box (notice s1 and plasma are selected).

- c. In the Variable for Y-Axis pane, click q1; q1 moves to the Current Selection pane.
- d. Press the CTRL key and click q2; q2 moves to the Current Selection pane. (Pressing the CTRL key allows you to select multiple items). The Plot and Table Variables dialog box will appear as shown below:

ex1 bolus	X-AXIS   t
ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1) olasma	Select up to 10 Y-Axis Variables in List. Current Selection :
q1 q2 s1 s1_res s1_wres t vol	q1 q2

e. Click **Done**. The plot will appear as follows:



f. With the Plot window open, in the Set menu click Plot/Table Variables. The Plot and Table Variables dialog box will open. Clear the List All Variables check box. In the Variables for Y axis pane, click s1:plasma, then click Done. The Plot window will appear as follows:



10. Fit the model to the data.

a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit** 



*Leaving the Plot window open.* The **Plot** window can remain open during a "Solve" or "Fit.". The plot will be updated after a successful "Solve" or "Fit."





*Fit status*. During a "Fit," a **Fit Status** message will appear (on a fast computer, you may just see a flash). This is the counterpart to the **Solution Status** message you saw when you solved the model originally. The **Fitting Status** bar gives information both on the integration part of the "Fitting" and on the number of iterations. You can abort the "Fit" by clicking **Abort**.



When you have Fitted the model to the data, the **SAAM II Compartmental** main window should appear with the **Plot** window as follows:



The new parameter values will replace the original estimates in the **Parameters** dialog box, and the best fit of the model to the data appears in the plot. (You can change the plot to semi-logarithmic if you wish by clicking **Semilog** in the **View** menu - this is possible because the **Plot** window is open.) The semilog plot will appear as follows:



- b. Change the variables plotted to s1\_wres, the weighted residuals for the fit.
  - i. On the SAAM II Toolbar, click Select Variables:



The **Plot and Tables Variables** dialog box will open. Check the **List All Variables** check box, and select **s1\_wres**, and de-select semilog:

ariables for Y-Axis	X-Axis t
ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1)	Select up to 10 Y-Axis Variables in List. Current Selection :
q1 q2 s1 s1_res s1_wres t	s1_wres
vol	

Click **Done**. The following plot will appear.



ii. Change the scale of the plot by clicking **Set scales** on the **SAAM II Toolbar**:



The Set Scales dialog box will open:

Axis	Minimum	Maximum
AutoScale	0.0	9.00000000
Set	0.0	9.00000000
AutoScale Set	-1.50706365	1.49422038

Click the **Set** radio button for the X Axis, and set the Maximum equal to 9.5; click the Set radio button for the Y axis, and set the Minimum and Maximum respectively equal to -2 and 2:

Minimum	Maximum
0.0	9.00000000
0.0	9.500
-2.000	2.000
	Minimum 0.0 0.0 -1.50706365 -2.000

Click **Done**. Your plot will be updated:



- iii. Return to your plot of plasma and model fit by using Select Variables on the SAAM II Toolbar, deselecting List All Variables, selecting s1:plasma, and clicking Done. Then change the scale by using Set Scales on the SAAM II Toolbar, setting both the X and Y-axis to AutoScale, and click Done.
- 11. View the statistics associated with the "Fit."
  - a. In the Show menu, click Statistics, or alternatively on the SAAM II Toolbar click
     Statistics Statistics window will appear as follows:

Statistics					
Parameter/Variable	Value	Std.Dev.	Coef. of Var.	95% Confidence	Interval
k(0,1)	0.29227	1.46155e-002	5.00071e+000	0.26010	0.32444 🔺
k(1,2)	0.28311	7.51183e-002	2.65335e+001	0.11777	0.44844
k(2,1)	0.17452	1.82636e-002	1.04652e+001	0.13432	0.21472
vol	2323.77661	3.85619e+001	1.65945e+000	2238.90219	2408.65103
C Correlation Matrix	C Covarian	ce Matrix 🔎	Objective		<u>.</u>
		Objective	Scaled Data V	ariance	
s1 : plasma	1.33674	3e+001	1.113515e-00	1	
Total objective	1.33674	3e+001			
AIC	7.93598	7e+000			



*Statistical information following a successful "Fit."* The **Statistics** window contains information about the "Fit." It includes

- i. the final values for the parameters, their estimated standard deviation, percent coefficient of variation, and 95% confidence interval.
- ii. the following objective function information:
  - Final value of the objective function (this is the function that is minimized during the fitting process)
  - Scaled data variance (this is a number that is estimated during the fitting process when you use relative weighting the default option in SAAM II)
  - Values for AIC and BIC; these values are used in the model development process to help assess which model structure best fits the data.
- iii. the Covariance matrix.
- iv. the Correlation matrix.

If, for example, in the **Statistics** window, you select the **Correlation Matrix** option, the Correlation Matrix will appear in the lower half of the **Statistics** window. The Covariance Matrix or the values for the Objective will appear if you select one of these other options.



- b. Close the **Statistics** window.
- c. Close the **Plot** window.

#### 12. Quit the SAAM II Compartmental application

- a. In the **File** menu, click **Exit**.
- b. Click **No** (you do not wish to save the file).

## Part 2. Building models and creating experiments in the SAAM II Compartmental application.

This part of the tutorial will show you how to build the two-compartment model and conduct the experiment on the model used in Part 1. This part of the tutorial will show you how to use the **Model** and **Experiment** tools in the **SAAM II Toolbox** for building system models and creating experiments on the models.

1. Start the **Compartmental** application. The **SAAM II Compartmental** main window will open as follows:

SAAM II Compartmental - UNTITLED	- O ×
File Edit View Show Compute Set Window Help	
Toolbox UNTITLED:1	
Model	
Select Compartment	
Delay Flux	
Experiment Name:	
Choose Rename	
Create Remove	
Select Gample	
Change	
Condition	
	4

- 2. Create the two compartments of the two-compartment model.
  - a. In the **SAAM II Toolbox**, click **Model**. (This ensures that the **SAAM II Model** building tools are available.)
  - b. In the **SAAM II Toolbox**, click **Compartment** (this tool is now available).
  - c. Click on the **Drawing Canvas** approximately where you would like the first compartment to be located. A compartment with the number **1** will appear on the **Drawing Canvas**.

- d. Click **Compartment** in the **SAAM II Toolbox** a second time (this tool is again available).
- e. Click on the **Drawing Canvas** approximately where you would like the second compartment to be located. A compartment with the number **2** will appear on the **Drawing Canvas**. The **SAAM II Compartmental** main window should appear as shown below:





Locking Tools. If you know you are going to be creating several compartments for the model, you can lock the **Compartment** tool so it is available until you unlock it. For example, to facilitate building a multi-compartmental model, you can do either of the following:

- i. In the SAAM II Toolbox, double-click Compartment to lock the tool, or
- ii. In the **SAAM II Toolbox**, click **Compartment**, and then select the **Lock** check box at the bottom of the **SAAM II Toolbox**.

The **Compartment** tool will be available until you unlock it by clicking **Select** in the **SAAM II Toolbox**.





*Objects and Dialog Boxes.* Remember, every object on the **SAAM II Compartmental Drawing Canvas** has a dialog box associated with it. Double-click compartment **1** to open the **Compartment Attributes** dialog box associated with this compartment. Type "Plasma" in the **Reference Name** box as shown below:

Compartment #	Attributes	×
Compartmen Referer	t Number: 1 nce Name: Pla	sma
Done	Cancel	Help

Click close the dialog box, click **Done**. Note the word "Plasma" appears in the circle that represents Compartment **1**.



- 3. Construct transfers between Compartments 1 and 2.
  - a. In the **SAAM II Toolbox**, double-click **Flux** (notice that double-clicking will lock the **Flux** tool so you can perform multiple operations).
  - b. On the **Drawing Canvas**, click on Compartment 1, then click on Compartment 2.

A flux (transfer) arrow to Compartment 2 from Compartment 1 that is labeled k(2,1) is created. If the label does not appear, it is because Compartments 1 and 2 are too close to each other. If this is the case, move Compartment 2 farther away from Compartment 1. Notice when you drag the **flux** tool towards Compartment 2, Compartment 1 is highlighted, and there is a dotted line showing where the flux is going:



c. On the **Drawing Canvas**, click on Compartment 2, and then click on Compartment 1.

A flux (transfer) arrow to Compartment 1 from Compartment 2 that is labeled k(1,2) is created.

d. In the **SAAM II Toolbox**, click **Select**. The **Flux** tool is no longer available. The **SAAM II Compartmental** main window should appear as shown below:

SAAM II Compartmental - UNTITLED	<u>- I ×</u>
File Edit View Show Compute Set Window Help	
Image: Compartment     Image: Compartment       Image: Choose     Rename       Rename     Rename       Rename     Rename       Rename     Rename       Rename     Rename       Rename	
Select model component NUM	

Notice, as described above, Compartment **1** has been given the reference name "Plasma."



*Creating transfers.* To create a transfer between, for example, Compartment 1 and 2, with the **Flux** tool available, you can click on Compartment 1 and drag to Compartment 2.



4. Construct losses from Compartments 1 and 2.

- a. In the SAAM II Toolbox, double-click Flux.
- b. On the **Drawing Canvas**, click on Compartment **1**, and then click anywhere on the canvas.

This will create a loss, k(0,1), from Compartment 1. No matter where you click on the **Drawing Canvas**, the loss will always point down.

c. On the **Drawing Canvas**, click on Compartment **2**, and then click anywhere on the canvas.

This will create a loss, k(0,2), from Compartment 2.

d. In the **SAAM II Toolbox**, click **Select**. The **Flux** tool is no longer available. The **SAAM II Compartmental** main window should appear as follows:





*Moving or nudging a compartment on the Drawing Canvas*. Suppose after you have created the model you want to move or nudge a compartment on the **Drawing** 

**Canvas** to line it up with another object. To move an object, click the compartment or delay you wish to move, and drag the object to where you would like it to be located on the **Drawing Canvas**. To nudge an object (e.g. to straighten transfer arrows), click the compartment you wish to nudge, and nudge it using the directional arrows on the keyboard.





*Correcting a mistake by deleting an object.* Suppose you accidentally add an object to the model by mistake. To delete the object from the **Drawing Canvas**:

- i. On the **Drawing Canvas**, click the object you wish to delete.
- ii. Either press the **Delete** key, or in the **Edit** menu, click **Delete**. The following warning message will appear as follows:



iii. Click **OK** if it is okay, otherwise click **Cancel**.





Deleted Objects. When a compartment or delay is deleted, all attached arrows, experimental samples and inputs are also deleted!



- 5. Delete the loss k(0,2) from the model.
  - a. On the **Drawing Canvas**, click k(0,2) to select it.
  - b. Press the **Delete** key.
  - c. Click OK.

This will delete the loss k(0,2) from the model.

At this point, you have successfully created the two-compartment system model with a single loss from Compartment 1 used in Part 1. You now want to reproduce the experiment performed in the laboratory on this model. This point emphasizes the difference between building the system model and creating an experiment on the model. Obviously, as you can see below, there are many different experiments that can be created on the model. The main differences are where and how inputs are made, and where and how samples are taken. Separating the system from the experiment permits maximum flexibility in using the tools in the **SAAM II Toolbox**.

- 6. Create the experiment.
  - a. In the **SAAM II Toolbox**, click **Experiment**. Notice that the **Model** tools are unavailable and the **Experiment** tools are available.

The Experiment Attributes	dialog box	will open	as follows:
---------------------------	------------	-----------	-------------

Independent Variable:	t
Units:	minutes
Start at:	0.0
End at:	1

- b. Change the entry in the Units box from "minutes" to "days."
- c. Enter "9" in the **End at** box. The **Experiment Attributes** dialog box will appear as shown below:

t
days
0.0
9
cel Help



*Experiment Attributes*. The **Experiment Attributes** dialog box is normally where you set the ending time of the experiment. **Units** are for convenience only. **Start at** is normally zero which is the time of the first test input. **End at** is normally the time at which the experiment ends. There are, however, occasions when you may wish to set **End at** to a larger value.



d. Click Done.

The **Create Experiment** dialog box will appear on the **Drawing Canvas**. The choice of experiment **Types** is an **Experiment** or a **System**. **Experiment** is selected. The **New Name** is "Exper" as shown in the following:

Create Experiment			
New Name:	Exper	5	
Type:	Experiment	System	
Create	Cancel	Help	

#### e. Click Create.



*Experiment vs. System.* The **Create Experiment** dialog box is where you create your experiment. There are two types of experiments - "Experiment" and "System".

The **Experiment** type will invoke SAAM II's differential equation machinery. When you create this type of experiment, your compartmental model will be interpreted by SAAM II as a system of differential equations. Once parameter values and inputs have been specified, SAAM II can Solve the system of differential equations, and can Fit your model to your data. This type of experiment is designed to deal with time dependent data following an experimental (exogenous) input into the system.

The **System** experiment creates a system of algebraic equations whose coefficients are the k(i,j) of your compartmental model. The System model is used primarily in tracer-trace experiments to describe the tracee data in the steady-state. How to use **System** models is not discussed here.

The default New Name is "Exper". This can be changed to a name of your choice.





f. The **SAAM II Compartmental** main window should appear as follows:



SAAM II Notation. Remember the model looks like the original model except now the compartment numbers have changed from 1 and 2 to q1 and q2. Here q1 and q2 represent the solutions to the differential equations q1' and q2' created internally by SAAM II. The q1 and q2 are the calculated masses of experimental inputs into the two compartments at time t.



To recreate your laboratory experiment on the model, you need to specify the site and amount of your experimental input, the site of your measurement, and specify the measurement equation.

- 7. Add an experimental input to the model.
  - a. In the SAAM II Toolbox, click Input.

b. On the **Drawing Canvas**, click Compartment **q1**, and then click on the canvas.

An input arrow named **ex1** will appear on the **Drawing Canvas** pointing to Compartment **q1**. The **SAAM II Compartmental** main window should appear as follows:



- c. Double-click ex1. The Exogenous Input dialog box will open.
- b. Enter "1.04e+08" in the **Initial Amount** box.
- e. Click **Add**. The **Exogenous Input** dialog box should appear as follows (this is identical to the **Exogenous Input** dialog box you viewed in Part 1):

ogenous 1	ínput					>
lame: ex1		Refe	rence		Units:	
Туре	Initial	Constant	Start	Stop	Repeat Every	Nr. Repeats
lolus	1.04e+	8 -	0.000	112	100	
Input Ty	pe:		Initial Am	ount: 1.0	) <del>4e+08</del>	Save
Bolu	s		Constant	Rate:		
C Infu C Prim	sion ed Infusion		Event	Start:		⟨⇒Edit⊅
C Equi	ation		Event	Stop:		
			Repeat E	very:		
			Nr. of Rep	eats:		Delete 🕹
Equation:	ex1 =				26	
Solit In	mut	E .	Do	ne	Cancel	Help

- f. Click Done.
- 9. Create a sample on the model. This sample will represent the sample you collected in your actual experiment.
  - a. In the SAAM II Toolbox, click Sample.
  - b. On the **Drawing Canvas**, click Compartment **q1**, and then click on the canvas.

A sample object, **s1**, will appear on the **Drawing Canvas** attached to Compartment **q1**. This means your sample was from plasma. Notice that the circle at the top of the sample object is an open circle. The sample object can be moved on the **Drawing Canvas** as described above.



The **SAAM II Compartmental** main window should appear as shown below:

c. On the **Drawing Canvas**, double-click **s1** to open the **Sample Attributes** dialog box as shown below:

Associate with Da	Name: s1 Units:    ta Name:	
Associate with Da	Units: 🛛 ta Name: 🔽	
Associate with Da	ta Name:	
	1	
	100	
uations:		
= q1		2
		13

d. Type "plasma" in the **Associate with Data Name** box. As discussed in more detail below, "plasma" is the name of the data in the data file.

e. Edit the sample equation "s1 = q1" to read "s1 = q1/vol" in the **Equations** pane. As discussed below, *vol* will become a new parameter in the model.



*The Sample Equation.* The sample equation, in this case "s1 = q1/vol", is what links the solution to the differential equations, the **q1** and **q2**, with the data. The units of the differential equations are determined by the units of the input, **ex1**. The units of your data are usually concentration. Thus the sample equation keeps the units of the differential equations and the units of the data consistent.



f. If you wish, you can type "dpm/ml" in the **Units** box; this will be for bookkeeping purposes only.

The **Sample Attributes** dialog box will appear as shown below:

<u>_</u>

g. Click **Done**. A warning message will appear because you have not entered your data yet. This warning message is shown below:



h. Click OK.



*Sample Attributes*. There are a number of important points to be made here that will help you when you use the **SAAM II Compartmental** application:

- i. When you close the **Sample Attributes** dialog box, you will get a warning message that the data element, i.e. the data named "plasma," does not exist yet. This is because you have not yet entered your data. If you had entered the data first, and your data contained a column named "plasma," you would not get this message.
- ii. The data name in **SAAM II** is case sensitive. Thus "Plasma" and "plasma" will be read as two different names.
- iii. The circle at the top of the Sample object will be solid when there is a data name associated with the sample. This is used as a modeling aid to help remind you when data associations were made.
- iv. The sample equation "s1 = q1/vol" introduced a new parameter *vol* for the volume of Compartment **q1**.



10. Add the data to the SAAM II Compartmental model.

The data you will use in **study\_0** are shown below. These are decaying data following the bolus injection of a radio-labeled protein. A plot of these data is shown below:



- a. On the Show menu, click Data, or alternatively, on the SAAM II Toolbar, click Data Data . The Data window will open.
- b. On the **File** menu, click **Open**. The file **study\_0.dat** should appear in the list (if it does not, find the folder where you put this data file).
- c. Double-click **study\_0**. The data in this file will appear in the **Data** window. The model and the **Data** window should appear on the **Drawing Canvas** as follows:



d. Close the **Data** window.



*Error structure of the data*. For this introductory tutorial, the errors in the data are assumed to be a constant coefficient of variation; in this case Fractional Standard Deviation (FSD); this is denoted in the data file by (*FSD 0.1*).



11. Enter the parameter values.

The parameters for the model are k(2,1), k(1,2), k(0,1) and vol.

a. In the **Show** menu, click **Parameters**, or alternatively, on the **SAAM II Toolbar** click **Parameters Parameters** dialog box will open as follows:

Name	Туре	Current	Low Limit	High Limit
k(0,1)	Adj	10	53	
k(1,2)	Adj			
k(2,1)	Adj			
vol	Adj			
Name:     k(0,1)     Value:       Type:     C     Eixed       Image: C     Eixed     Low Limit:       Image: Adjustable     High Limit:				Edit - D :ave 소

The parameter k(0,1) should be selected. If it is not selected, double-click k(0,1) to select it. Be sure the **Adjustable** button is selected.

b. Enter "0.1" in the **Value** box, and click **Save**.



*Default low and high parameter limits*. Notice that when a value is entered in the **Value** box and nothing is entered in the **Low Limit** or **High Limit** boxes, the default low and high limits of one tenth of the value and ten times the value respectively are automatically entered when the value is saved.



- c. Double-click k(1,2) to select it.
- d. Enter "0.1" in the Value box, and click Save.
- e. Double-click k(2,1) to select it.
- f. Enter "0.1" in the **Value** box, and click **Save**.

- g. Double-click vol to select it.
- h. Enter "2000" in the Value box, and click Save.

When you have finished, the **Parameters** dialog box should appear as follows:

Name	Туре	Current	Low Limit	High Limit
k(0,1)	Adj	0.1000	0.0100	1.0000
k(1,2)	Adj	0.1000	0.0100	1.0000
k(2,1)	Adj	0.1000	0.0100	1.0000
vol	Adj	2000.0000	200.0000	20000.0000
Name: vol Type: O Eixed O Adjustable	Valu Low Lim High Lim	e: 2000 it: 200.00000 it: 2000.0000		□Edit⊅ Save♪

i. Click Done.



*Single or double-clicking a parameter in the Parameters dialog box.* When the **Parameters** dialog box is open, there is always a current parameter. Its name appears in **Name:** in the lower pane. The **Value, Low Limit** and **High Limit** boxes will either contain the values associated with the current parameter or be empty if no values have been entered.

If you single-click on another parameter, the **Name** of the current parameter will not change nor will the entries in the **Value**, **Low Limit** and **High Limit** boxes. However, if you click **Save**, the current **Value**, **Low Limit** and **High Limit** shown in the boxes will be saved for the new parameter. This makes it easy to enter the same values for more than one parameter. If you double-click on another parameter, the name of the new parameter will appear in **Name:**. The **Value**, **Low Limit** and **High Limit** boxes will change to the values associated with this parameter. If no values were entered for this parameter, these boxes will be cleared, and you can enter the new values for this parameter.



You have now successfully created the model used in Part 1 of the tutorial.

#### 12. Quit the SAAM II Compartmental application.

- a. In the **File** menu, click **Exit**.
- b. Click No.

### Data for this tutorial

DATA	L			
(FSD 0.1)				
t	plasma			
0.007	46780			
0.042	43522			
0.125	42535			
0.25	40125			
0.375	36221			
0.5	35562			
1.0	28194			
2.0	19573			
3.0	14403			
4.0	11278			
5.0	8081			
6.0	6999			
7.0	5653			
8.0	5139			
9.0	4210			
END				